# A kinetic model of the central carbon metabolism for acrylic acid production in *Escherichia coli*

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## 1 – Introduction

Acrylic acid (AA) is predominantly used in the production of superabsorbent polymers, hence its worldwide demand and commercial value in the industrial business [1]. This chemical can be obtained by three main routes, through the oxidation of propylene and propane, through semi-biological methods like the 3-hydroxypropanoate (3-HP) and the lactic acid routes (LA), and through a bio-based route from a simple carbon source [2].

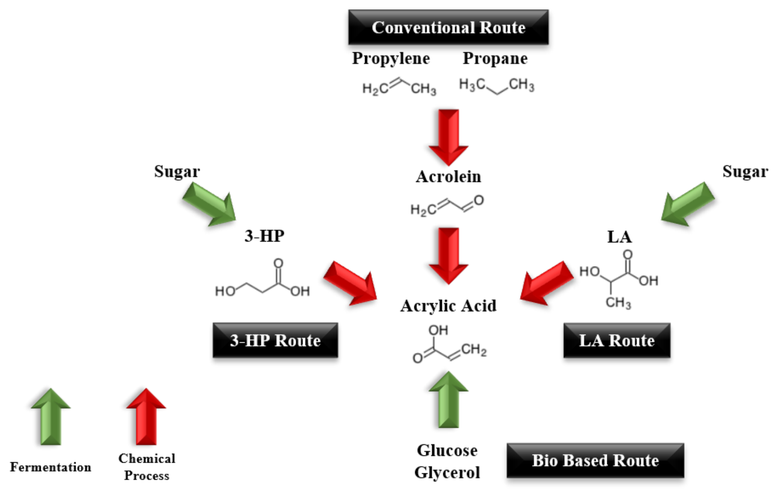


**Figure 1.** Routes for acrylic acid production.

The bio-based direct route represents a cheaper, innovative and cleaner method for AA production, although up to now it presents low yields [1, 2].

## 2 – Materials and Methods

Identify the pathways for AA production → Retrieve kinetic information of the reactions → Insert the pathways into a dynamic model of *E. coli* K-12 MG1655 central carbon metabolism → Perform time course simulations using COPASI

## 3 – Pathways for acrylic acid production

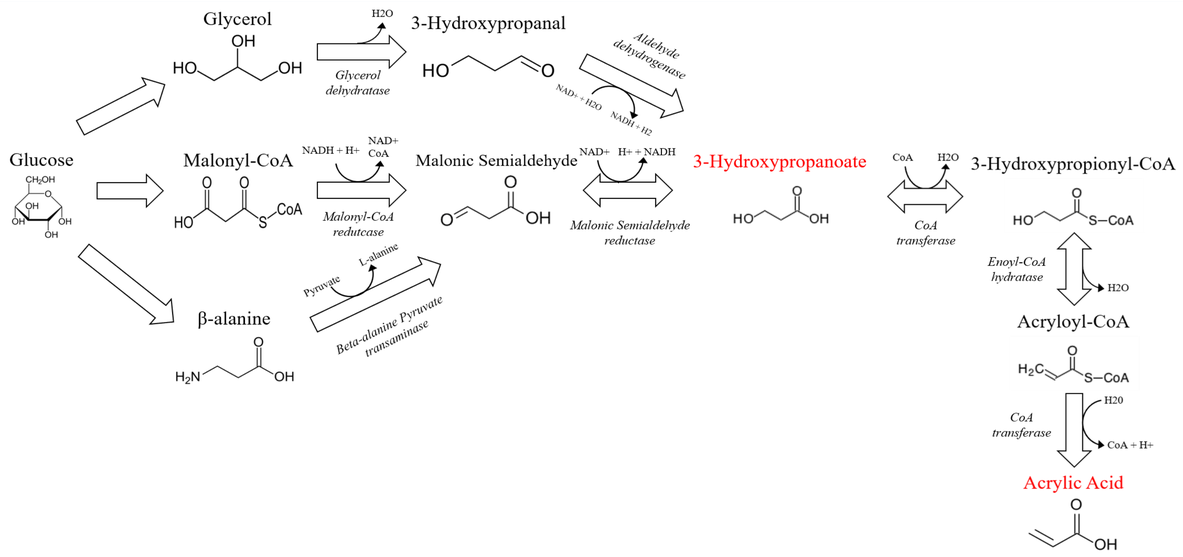


**Figure 2.** Identified pathways that lead to a bio-based acrylic acid production.

Although three distinct pathways were identified, only the glycerol route was tested in this work.

## 4 – Results and Discussion

After inserting the heterologous pathway into the kinetic model of Millard et al. [3], time course simulations were performed to access 3-HP and AA production in one hour. Within this time period, 0.043 mmol/l of 3-HP were accumulated, and a total of 7.73 mmol/l of AA were produced.

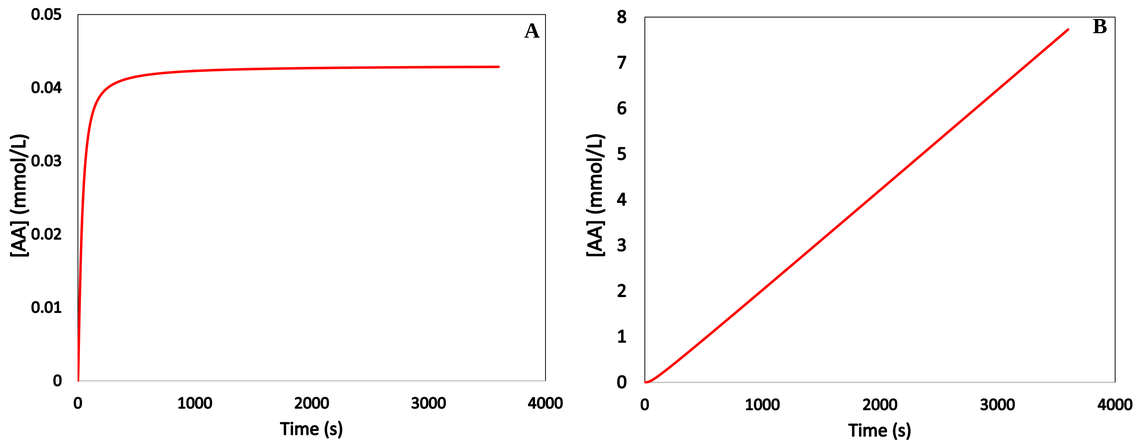


**Figure 3.** Predicted variation of concentration over time for 3-HP (A) and for AA (B).

Nevertheless, some problems have arisen in this work that may have influenced the yields of AA, namely:

- ✓ Glycerol was not present in the model.
  - Further work is needed to complement the model with reactions that include the consumption of glycerol in *E. coli.*
- ✓ Lack of kinetic data.
  - Enzymes such as glycerol dehydratase and CoA transferases were replaced by enzymes that perform similar reactions.
  - Reversibility of reactions, activating compounds, inhibitors, and toxic metabolites were not considered in this preliminary work.

## 5 – Conclusions and Future Work

- ✓ AA production was archived for the glycerol route.
- ✓ **Future work:**
  - Test the β-alanine and malonyl-CoA pathways to compare results;
  - Enrich the model with reactions that deflect the intermediates from AA production, and with the kinetic properties mentioned before;
  - Identify possible optimization strategies.

## References

[1] Chu H, Ahn J, Yun J, Choi I, Nam T, and Cho K. Direct fermentation route for the production of acrylic acid. Metabolic Engineering, 32:23–29, 2015.

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[3] Millard P, Smallbone K, and Mendes P. Metabolic regulation is sufficient for global and robust coordination of glucose uptake, catabolism, energy production and growth in *Escherichia coli*. PLoS computational biology, 13(2):e1005396, 2017.

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